

# 2,3,4,6,9-pentachlorodibenzofuran

**Other names:** Dibenzofuran, 2,3,4,6,9-pentachloro  
**Inchi:** InChI=1S/C12H3Cl5O/c13-5-1-2-6(14)12-8(5)4-3-7(15)9(16)10(17)11(4)18-12/h1-3H  
**InchiKey:** VANGHZRYKXDPRR-UHFFFAOYSA-N  
**Formula:** C12H3Cl5O  
**SMILES:** Clc1cc2c(oc3c(Cl)ccc(Cl)c32)c(Cl)c1Cl  
**Mol. weight [g/mol]:** 340.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2511.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2482.00		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	2511.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R29720&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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